

Flux qubits shed a new light on BCS theory and high- T_c superconductivity

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Abstract

A simple microscopic model of a small superconducting loop interrupted by Josephson junction (flux qubit) allows to compute from the experimental data of Wal et.al [1] an important parameter - the density of Cooper pairs at zero temperature. This density is determined by the cut-off energy in the BCS model and agrees with the original BCS suggestion but is lower by two orders of magnitude than the value accepted in the modern literature. The immediate consequences of this result are: the validity of the strong coupling BCS model, a plausible picture of electrons recombination into Cooper pairs, and a much weaker condition for the appearance of high-temperature superconductivity. Another consequence is that the popular interpretation of Josephson qubits as macroscopic quantum systems is replaced by a picture of qubit states being superpositions of the ground state and the state containing only a single excited Cooper pair.

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Fifty years after the discovery of superconductivity Bardeen, Schrieffer, and Cooper (BCS) presented a theory of this phenomenon which remained valid for the next fifty years [2]. The BCS theory contains a cut-off energy parameter determining the number of electrons participating in the pairing mechanism and initially suggested to be comparable to the superconducting gap. For many years this parameter remained unspecified [3] but in the modern literature has been replaced by the Debye energy [4] which is about hundred times higher than the gap. The relatively new experiment with flux qubit [1] sheds a new light on that issue supporting the original hypothesis. The detailed analysis of the microscopic Hamiltonians based on this hypothesis is presented in [5] for all three types of Josephson qubits (charge, phase, and flux qubits [6]). Here, only a simplified model of flux qubit is discussed.

A flux qubit (FQ) is a small superconducting ring interrupted by one or several Josephson junctions. The thickness of the ring is assumed to be not larger than the penetration depth for the magnetic field (typically $\sim 100nm$), what allows to ignore spatial variations of the electric current density. The Cooper pair's circular states $|k, \mu\rangle$, which produce current, are labeled by two quantum numbers. The first one $k = 1, 2, \dots, K$ describes a Cooper pair in its center of motion reference frame and corresponds to a pair of time-reversed single electron states $|k_{\pm}\rangle$. Under standard half filling condition there are $K/2$ Cooper pairs in the sample at zero temperature. The second quantum number $\mu = 0, \pm 1, \pm 2, \dots$ accounts for the quantized circular motion of the Cooper pair along the ring. According to the Onsager hypothesis [7] a single Cooper pair in a state $|k, \mu\rangle$ generates a quantized magnetic flux $\mu\Phi_0$ where $\Phi_0 = h/2e$. Consider a configuration of Cooper pairs described by the occupation numbers $n_{k\mu}$ which take values 0, 1, as Cooper pairs behave like *hard core bosons*. The total magnetic flux is equal to $F\Phi_0$, where $F = \sum_{k,\mu} \mu n_{k\mu}$, and the magnetic energy of such configuration is given by

$$\mathcal{E}_M = E_L \left(\sum_{k,\mu} \mu n_{k\mu} \right)^2. \quad (1)$$

where

$$E_L = Kh^2/4m\ell^2, \quad (2)$$

m is electron's mass and ℓ is the length of the loop. The formulas (1) and (2) are derived using the London's relation between superconducting current density and vector potential $\mathbf{j} = -\frac{\mathcal{N}e^2}{m}\mathbf{A}$, the formula for the energy of a current in a magnetic field $\mathcal{E} = -\int \mathbf{j} \cdot \mathbf{A} d^3\mathbf{x} = \frac{K\epsilon^2}{m}A^2$ and the Onsager's magnetic flux quantization condition $\Phi = \oint \mathbf{A} \cdot d\mathbf{x} = \pm A\ell = F\Phi_0$, $F = 0, \pm 1, \pm 2, \dots$. Here, \mathcal{N} is a density of superconducting electrons and A denotes $|\mathbf{A}|$. Both quantities are assumed to be uniform in the sample what is true for thin enough loops (thickness $\leq 100nm$).

For loops of micrometer diameters, used to construct flux qubits, E_L is much higher than the superconducting gap what means that the states with different fluxes $F\Phi_0$ are separated by large energy gaps in comparison with the other relevant energy scales for the system. To produce a qubit one has to switch on an external flux $\Phi_{ext} = \mu_{ext}\Phi_0$ which modifies the magnetic energy yielding

$$\mathcal{E}_M(\mu_{ext}) = E_L(F - \mu_{ext})^2. \quad (3)$$

Taking $\mu_{ext} \simeq 1/2$ one can reduce the magnetic energy difference $\delta\mathcal{E}_M = E_L|1 - 2\mu_{ext}|$ between the unique ground state $|0\rangle$ with a flux $F = 0$ and the excited levels with $F = 1$. The stable states of a superconducting ring correspond to collective states of Cooper pairs with various flux population numbers $N_\mu = \sum_k n_{k\mu}$ such that $\sum_\mu N_\mu = K/2$. In particular the ground state $|0\rangle$ has the total flux equal to zero with N_μ concentrated around $\mu = 0$. The stable states with $F = 1$ are obtained from the ground state by changing the populations $N_\nu \mapsto N_\nu - 1, N_{\nu+1} \mapsto N_{\nu+1} + 1$ at the given ν . Such states are denoted by $|0, \nu\rangle$. The presence of Josephson junction(s) does not produce transitions between $|0\rangle$ and $|0, \nu\rangle$ because those states have a global and collective character while the Josephson junction should be described by a localized Hamiltonian perturbation \hat{V}_J . However, the transitions exist between $|0\rangle$ and the states $|0, \nu, k\rangle$ obtained from $|0, \nu\rangle$ by replacing one *ground pair* with the indices $(\nu + 1, k)$ by an *excited pair*. Excited Cooper pairs appear already in the original BCS paper [2] and possess a clear interpretation in terms of permutational symmetry within a strong-coupling BCS model [8]. The corresponding transition amplitudes $\xi_{\nu k} = \langle 0, \nu, k | \hat{V}_J | 0 \rangle$ determine the state

$$|1\rangle = \sum_{\nu, k} \tilde{\xi}_{\nu k} |0, \nu, k\rangle, \quad \tilde{\xi}_{\nu, k} = \frac{\xi_{\nu k}}{\sqrt{\sum_{\nu' k'} |\xi_{\nu' k'}|^2}} \quad (4)$$

which becomes separated from the others and together with the ground state $|0\rangle$ span the flux qubit Hilbert space.

In the two level approximation the eigenstates of the qubit Hamiltonian are suitable superpositions of $|0\rangle$ and $|1\rangle$ and the corresponding qubit frequency reads

$$f = \frac{1}{h} \sqrt{[E_L(1 - 2\tilde{\mu}_{ext})]^2 + E_J^2}. \quad (5)$$

Here, the Josephson energy $E_J = \sum_{\nu k} |\xi_{\nu k}|^2$ and $\tilde{\mu}_{ext} = \mu_{ext} + \delta$. The correction δ accounts for the fact that the excited pairs have higher energy than the ground ones (see [5] for the details).

The simple theory presented above can be now compared with the experiment of van der Wal et.al.[1]. The sample is an aluminum $5\mu m \times 5\mu m$ loop made of $450nm$ wide and $80nm$ thick lines. The Josephson junction loop is kept at the milikelvin temperatures and excited by the

microwave radiation with frequencies in the range of $1 - 10\text{GHz}$. The measured dependence of the resonant frequency on the control parameter $\tilde{\mu}_{ext}$ in the range $0.495 \leq \tilde{\mu}_{ext} \leq 0.505$ can be used to test the formula (5). The off-set δ is observed also, but attributed to persistent currents. The linear dependence on $|1 - 2\tilde{\mu}_{ext}|$ far enough from $\tilde{\mu}_{ext} = 1/2$ is clearly visible as well as the level repulsion for $\tilde{\mu}_{ext}$ very close to $1/2$ (see FIG.1). From those data the value $E_L/h \simeq 1.5 \times 10^3\text{GHz}$

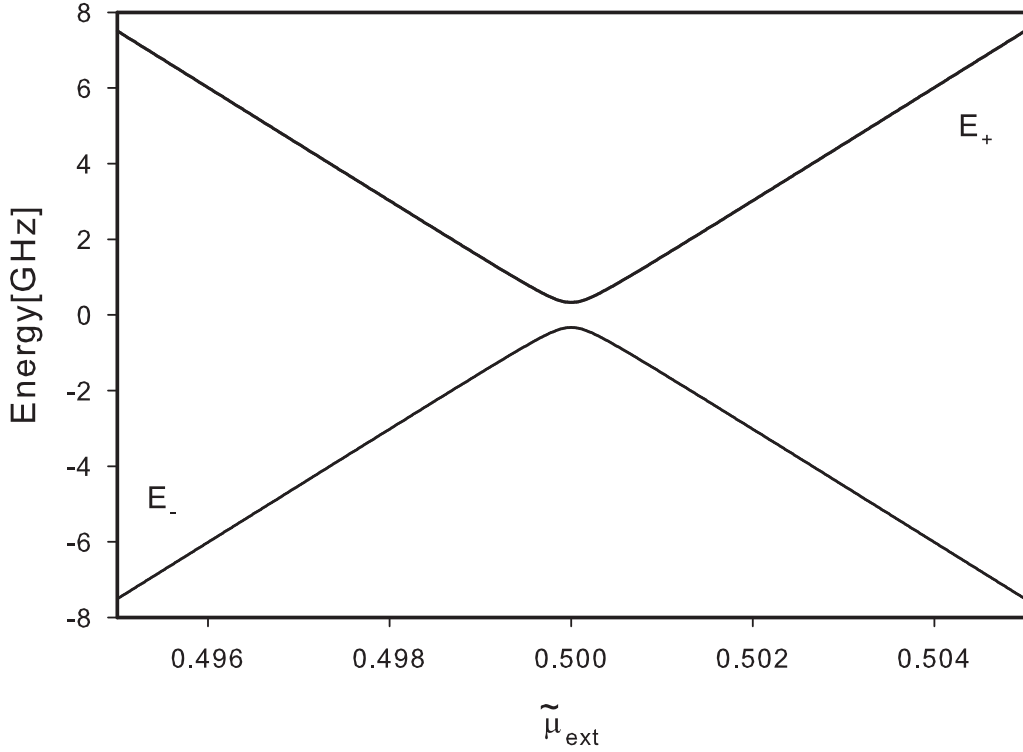


FIG. 1. Energy levels of the flux qubit (in GHz) as functions of the external magnetic flux (in Φ_0 units) given by (5). A fit to the data of van der Wal et.al. with $E_L/h = 1500\text{GHz}$ and $E_J/h = 0.66\text{GHz}$.

is extracted. Putting $\ell = 20\mu\text{m}$ into (2) one obtains $K = 3.3 \times 10^6$. The volume of the sample $\mathcal{V} = 0.72 \times 10^{-12}\text{cm}^3$ and hence, for the first time, one can compute directly from the experimental data the zero temperature density of Cooper pairs in a superconductor (Al)

$$\kappa_{CP}[\text{Al}] = K/2\mathcal{V} = 2.5 \times 10^{18}/\text{cm}^3. \quad (6)$$

The obtained result can be discussed within the BCS theory [2, 4]. The basic predictions of the BCS concern the relations between the superconducting gap at zero temperature $\Delta(0)$, the critical temperature T_c , the coupling constant g describing the magnitude of electron-phonon interaction

[9], and the cut-off parameter $\hbar\omega_c$

$$\Delta(0) = 1.76 k_B T_c, \quad k_B T_c = 1.13 \frac{\hbar\omega_c}{2 \sinh(\hbar\omega_c/g)}. \quad (7)$$

The energy cut-off $\hbar\omega_c$ limits the kinetic energy of the electrons participating in the BCS pairing mechanism to the interval $[E_F - \hbar\omega_c, E_F + \hbar\omega_c]$ (E_F - Fermi energy) and determines the number K of the corresponding electronic states by the expression [4]

$$K = 2\hbar\omega_c N(0). \quad (8)$$

Here, $N(0)$ is the density of electronic Bloch states (excluding electron's spin) at the Fermi surface given by [10]

$$N(0) = \mathcal{V} \frac{m}{2\pi^2 \hbar^2} (3\pi^2 \kappa_{el})^{1/3} \quad (9)$$

where κ_{el} is a density of electrons ($\kappa_{el}[Al] = 18.06 \times 10^{22}/\text{cm}^3$). After substitution one obtains $\hbar\omega_c/2k_B = 1.3K$ what is close to the critical temperature $T_c = 1.2K$ for *Al*. It allows to formulate the following hypothesis concerning the parametrization of the BCS model:

$$\hbar\omega_c \simeq g \simeq \Delta(0) \simeq 2k_B T_c. \quad (10)$$

Notice that (10) agrees with the suggestion $\hbar\omega_c \sim k_B T_c$ in the original BCS paper, as well as with the BCS relations (7). On the other hand the assumption $\omega_c = \omega_D$ (Debye frequency) usually made in the modern literature implies

$$\hbar\omega_c = \hbar\omega_D \gg g \gg \Delta(0) \simeq 2k_B T_c. \quad (11)$$

The choice $\hbar\omega_c \simeq g$ allows to replace the electron kinetic energy in the BCS Hamiltonian by a constant E_F what leads to a much simpler exactly solvable model which predicts the relation $g = \Delta(0) = 2k_B T_c$ [8].

Another consequence of (10) is the following plausible picture of electrons recombination into Cooper pairs. For the temperatures $T > T_c$ only about $4k_B T N(0)$ [11] electrons are thermally excited and contribute to specific heat and conductivity; the rest is "frozen in the Dirac sea". At the temperature T_c those $4k_B T_c N(0) = 2\hbar\omega_c N(0) = K$ electrons begin to recombine such that at zero temperature all of them form $K/2$ Cooper pairs while the rest of electrons remain frozen all the time.

The next consequence of (10) is presented on FIG.2 which shows the relations between the coupling constant g and the critical temperature T_c under the hypothesis (10) and (11), respectively.

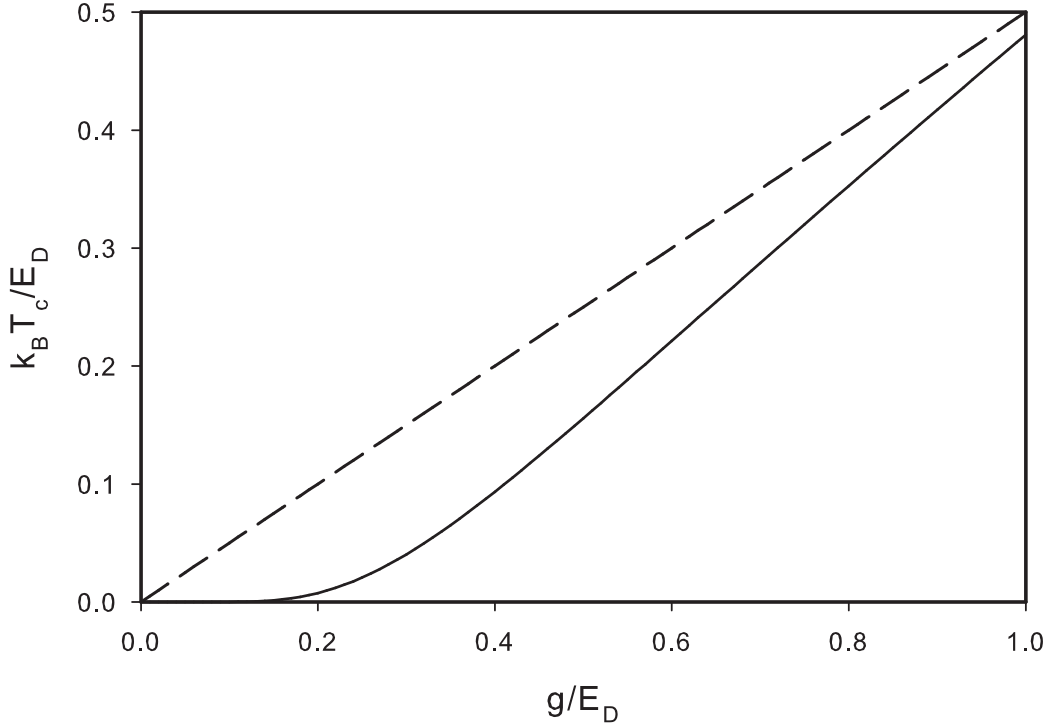


FIG. 2. Critical temperature as a function of the coupling constant (in Debye energy units $E_D = \hbar\omega_D$) for $k_B T_c = 1.13 E_D / 2 \sinh(E_D/g)$ (solid line) and $k_B T_c = g/2$ (dashed line).

Obviously, (10) allows to obtain quite high critical temperatures at the cost of moderate increase of the electron-phonon coupling, while (11) strongly suppresses the increase of T_c . For example, to obtain the critical temperatures $1.2K(Al)$ and $9.8K(Nb)$ one needs, assuming (11), the coupling constant g/k_B equal to $72K$ and $80K$, respectively. The same values of g , assuming (10), yield critical temperatures $36K$ and $40K$. Therefore, (10) suggests that the phonon-mediated pairing mechanism could be sufficient to explain high-temperature superconductivity, at least for a certain class of such materials [12].

In conclusion, it has been shown that the experimental results for a small Josephson junction loop interpreted in the light of the presented model do not only support the original BCS parametrization, what can be relevant for the theory of high-temperature superconductivity, but also change the physical picture of a flux qubit itself. Instead of the standard interpretation in terms of two macroscopic quantum states corresponding to the motion of millions of Cooper pairs, here the qubit's basis consists of the ground state and the state which differs from the ground one by a single excited pair, only. Obviously, more experimental evidence concerning flux qubits of

different sizes and made of different materials is needed as well as the first principle theoretical justification of the hypothesis (10).

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